THEOCHEM, VOLUME 61 (1989)

(*Journal of Molecular Structure, Vol. 202*)

AUTHOR INDEX

Angonoa, C., 203

Bachs, M., 315
Balasubramanian, K., 291
Berkowitz, J., 363

Chandra, A.K., 249
Cho, H., 363
Csavinszky, P., 337
Cvitaš, T., 227

Darakjian, Z., 111
Durig, J.R., 143, 159

Elabsy, A.M., 337

Fink, W.H., 111
Fulde, P., 63

Gibson, S.T., 363
Gunde, R., 325
Günthard, Hs.H., 325

Henry, B.R., 193
Hope, H., 111

Illas, F., 315

Jug, K., 277

Klasinc, L., 227
Klessinger, M., 129
Kovač, B., 227
Kovačević, K., 75
Kutzelnigg, W., 11

Little, T.S., 143

Macias, A., 235
Maksić, Z.B., 75, 265
Martin, F., 235
Mayhew, C.A., 363
Mo, O., 235

Nicolaides, C.A., 285
Nyulaszi, L., 227

Ōsawa, E., 169

Papadopoulos, M.G., 121
Pavlović, M., 265
Petrongolo, C., 135
Phan, H.V., 143
Primorac, M., 75
Ptak, W.S., 91

Qtaitat, M.A., 159

Reffy, J., 227
Ricart, J.M., 315
Riera, A., 235
Rubio, J., 315
Rudziński, J.M., 169
Ruscic, B., 363

Scheiner, S., 177
Schirmer, J., 203
Slanina, Z., 169
Smith, R.W., 347
Smith Jr., V.H., 347
Sokolić, F., 265
Sullivan, J.F., 159
Supek, I., 1
Swanton, D.J., 193
Szpunar, B., 347

Tkacz, K., 91
Todd, J., 99
Togasi, M., 169
Tomasello, P., 213

Van der Veken, B.J., 143
Veszpremi, T., 227
Von Niessen, W., 213

Waite, J., 121
Whitehead, M.A., 99

Yañez, M., 235

Zsombok, G., 227

THEOCHEM, VOLUME 61 (1989)

(Journal of Molecular Structure, Vol. 202)

SUBJECT INDEX

Abrupt heterojunctions
Effective-mass Hamiltonians and wave-function-matching conditions for abrupt heterojunctions, 337
Aluminum
Growth of small silicon and aluminum clusters, 277
Autoionizing states
A new method to calculate lifetimes of atomic and molecular autoionizing states, 235

Chemisorption cluster model
Taking into account non-dynamical correlation effects in ab initio chemisorption cluster model calculations, 315
Chloroacetaldehye
Conformational analysis and structural determinations from ab initio calculations for chloroacetaldehyde, 143
Coinage metal clusters
Electronic structure of coinage metal clusters, 291
Collinear reactions
MRD-CI quartet potential surfaces for the collinear reactions N $(^4S_u)+N_2(X^1\Sigma_g^+$, $A^3\Sigma_u^+$, *and* $B^3\pi_g)$, 135

(123) and (2212) copper oxides
Magnetism and electronic structure in the (123) and (2212) copper oxides, 347
Correlations
Treatment of electron correlations by local operators: a status report, 63

Dimethyl-γ-pyrone
Comparison of X-ray and ab initio deformation densities in dimethyl-γ-pyrone and triazine trichloride, 111

Electronic structure
Electronic structure and properties of molecules in excited states, 129
Excited clusters
Chemically bound excited clusters, 285
Excited states
Electronic structure and properties of molecules in excited states, 129
Excited-state structures
Excited-state structures of molecules with nearby electronic states, 249

Fues potential
Electron density for atoms from Fues potential within *H–K–S* theory, 91

Giant molecules
Quantum-chemically supported vibrational analysis of giant molecules: the C_{60} and C_{70} clusters, 169

H–K–S theory
Electron density for atoms from Fues potential within *H–K–S* theory, 91
Hermite–Gaussian expansion
Appraisal of Hermite–Gaussian expansion of hydrogen orbitals by calculation of some one-electron properties, 75
Hydrogen bonded systems
Ab initio studies of the structure, energetics and vibrational spectra of hydrogen bonded systems, 177

Inner valence photoelectron spectra
Inner valence photoelectron spectra - from qualitative to quantitative results, 213

Lifetimes
A new method to calculate lifetimes of atomic and molecular autoionizing states, 235
Local operators
Treatment of electron correlations by local operators: a status report, 63
Local-mode overtone spectra
The frequency–bond length correlation in local-mode overtone spectra, 193
Localized electronegativity group orbital
The localized electronegativity group orbital (LEGO): group hardnesses for acids and bases theory, 99

Molecular properties
Ab initio calculation of molecular properties, 11
Molecule–matrix interactions Structure, energetics and molecule–matrix interactions of molecules substituted into inert clusters and crystals: consistent force field treatment of substitutional defects in imperfect matrices: *trans*-1,2-difluoroethane: Ar_{363}, 325
MRD-CI quartet potential surfaces
MRD-CI quartet potential surfaces for the collinear reactions $N(^4S_u)+N_2(X^1\Sigma_g^+$, $A^3\Sigma_u^+$, and $B^3\pi_g$), 135

Non-dynamical correlation effects
Taking into account non-dynamical correlation effects in ab initio chemisorption cluster model calculations, 315

One-electron properties
Appraisal of Hermite–Gaussian expansion of hydrogen orbitals by calculation of some one-electron properties, 75

Photoionization studies
Bonding and structure in the hydrides of groups III–VI deduced from photoionization studies, 363
Polarisability
On the effect of conjugation and charge transfer on the polarisability, first and second hyperpolarisabilities of some polyenes and nitropolyenes, 121
Polyenes,
On the effect of conjugation and charge transfer on the polarisability, first and second hyperpolarisabilities of some polyenes and nitropolyenes, 121

Rudjer Bošković:
Rudjer Bošković: anticipation of modern science, 1

Silicon
Growth of small silicon and aluminum clusters, 277
SO_2 molecules
Distributed atomic multipole moments and intermolecular potentials: test calculations of the second virial coefficient of the SO_2 molecule, 265
Substituent effect of halogens
Photoelectron spectroscopy study of substituent effect of halogens on the thiophene ring, 227
Substitutional defects
Structure, energetics and molecule–matrix interactions of molecules substituted into inert clusters and crystals: consistent force field treatment of substitutional defects in imperfect matrices: *trans*-1,2-difluoroethane: Ar_{363}, 325

Thiophene rings
Photoelectron spectroscopy study of substituent effect of halogens on the thiophene ring, 227
Triazine trichloride
Comparison of X-ray and ab initio deformation densities in dimethyl-γ-pyrone and triazine trichloride, 111

Vinyl silyl chloride
Conformational analysis and structural determinations from ab initio calculations for vinyl silyl chloride, 159
Virial coefficient
Distributed atomic multipole moments and intermolecular potentials: test calculations of the second virial coefficient of the SO_2 molecule, 265